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The Boltzmann equation in the difference formulation

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Abstract

First we recall the assumptions that are needed for the validity of the Boltzmann equation and for the validity of the compressible Euler equations. We then present the difference formulation of these equations and make a connection with the time-honored Chapman - Enskog expansion. We discuss the hydrodynamic limit and calculate the thermal conductivity of a monatomic gas, using a simplified approximation for the collision term. Our formulation is more consistent and simpler than the traditional derivation.

Key words:

1 Introduction

The Boltzmann equation is based on a picture of N point-like particles. They evolve in time by Newton's equations and they interact with each other. In the "particle" picture, in 3D space, they are characterized by a distribution function in $6N$ dimensions. There is an intermediate stage of the Boltzmann equation, in terms of the single particle density in 6 dimensional phase space (coordinates and velocities). This is usually called a "kinetic" or mesoscopic picture. The kinetic picture is valid if two basic conditions are met: the interaction range of the particles is small with respect to their mean free path; and the particles entering a collision have random directions and velocities. These assumptions ensure that three-body and higher correlations can be neglected. Therefore dense fluids and boundary layers within the mean free path are explicitly excluded.

By "straightforward" theory in the low Knudsen number limit (Kn = the ratio of the effective range of the collisions to the mean free path), the compressible Euler equations are obtained, but the equation of state is always that of an ideal gas.

Hydrodynamics is based on a picture of continuous matter. At each point there is a density and a velocity vector with no accounting for the distribution of molecular velocities. Hydrodynamics breaks down in the vicinity of shock waves and fluid boundaries and it has to use phenomenological transport coefficients. Also, it does not include fluctuations in the parameters.

In this paper we do a simple transformation of the Boltzmann equation. We split the single particle density in space and velocity, $f(\mathbf{r}, \mathbf{v}, t)$, into a sum of a Maxwellian velocity distribution at each point in space and a “difference” velocity distribution - in a manner similar to the difference formulation of radiation transport [1]. The Maxwell part satisfies equations that are similar to the hydrodynamic equations and it is a source for the difference term.

From our work on radiation transport we know that in optically thick regions the radiation approaches Planckian and the difference field gets very small. We expect that in regions where the gradients are small the difference distribution will also get small (after some relaxation time). In fact, in our experience with real-life radiation transport problems, it has become clear that in optically thick media the difference formulation of radiation transport produces the same result as the diffusion equation. Furthermore, it always satisfies the correct boundary conditions, provided the discretization in space and time is done properly.

There are recent papers on treating some parts of fluids and gases by the Boltzmann equations and other parts by hydrodynamics [2],[3]. In these approaches there are difficulties in establishing consistent boundary conditions at the interface between the particle and hydrodynamic treatments. We hope that the new formalism will improve these calculations. It should also provide a significant speedup of them. Other hopes are that one can seamlessly couple molecular dynamics with a continuum description of diffusion phenomena. We also hope that our work will point to a new, and more consistent way of deriving transport coefficients. We also hope that someone will extend the treatment to non-ideal fluids.

2 Background

In this section, we present a very brief review of the background material for the rest of the paper. Our derivation is similar to that of Esposito, Lebowitz and Marra (ELM) [4], but we use some of the notation of Liboff (LIB) [5]. It sets the stage for the next section where, inspired by the difference formulation of radiation transport [1], we separate the “mesoscopic” Boltzmann kinetic equation into a local Maxwellian velocity distribution and a deviation.

We use $f(\mathbf{r}, \mathbf{v}, t)$ for the time-dependent six-dimensional particle density. We will call it the local velocity distribution function of the particles. We denote by $M(\mathbf{r}, \mathbf{v}, t)$ the local Maxwell distribution and use $\mathbf{F}(\mathbf{r}, t)$ for the volume force.

The Boltzmann equation (ELM 1.1), (LIB 3.2.14) for the distribution function is

$$\frac{\partial f(\mathbf{r}, \mathbf{v}, t)}{\partial t} + \mathbf{v} \cdot \nabla_x f + \mathbf{F} \cdot \nabla_v f = Q(f, f) \quad (1)$$

$Q(f, f)$ is the collision operator. The two gradients, ∇_x and ∇_v are those in real and velocity space.

We will use a component notation. We use i, j, k for any three orthogonal components of space and velocity. We also use the Einstein convention of summation over repeated indices. The Boltzmann equation becomes

$$\frac{\partial f(\mathbf{r}, \mathbf{v}, t)}{\partial t} + v_j \frac{\partial f}{\partial x_j} + F_j \frac{\partial f}{\partial v_j} = Q(f, f) \quad (2)$$

The equation assumes homogeneity of the one-particle distribution function over the collision volume, molecular chaos of the incoming particles, no multiple collisions and no second order correlations of $f(\mathbf{r}, \mathbf{v}, t)$. These assumptions have been discussed widely in the literature. We do *not* want to contribute to the discussion; we agree with everybody, even if some of them seem to contradict one another.

There are “collisional invariants” of the collision operator. These are consequences of the fact that individual elastic collisions of point-like particles conserve the number of particles as well as energy and momentum. Consider two distributions, $f(\mathbf{v})$, $g(\mathbf{v})$ of one particle velocity. Their evolution by collisions is given by $Q(f, g)$. If a quantity $\psi(\mathbf{v})$ is a collisional invariant, i.e. it is not changed by collisions, the integral of $Q(f, g)$ over a conserved $\psi(\mathbf{v})$ has to vanish. This is expressed as

$$\int Q(f, g) \psi(\mathbf{v}) d\mathbf{v} = 0 \quad (3)$$

Here $d\mathbf{v} = dv_i dv_j dv_k$ is the product of (any) three orthogonal spatial components of the velocity.

Now we write down the local conservation laws. They are *not* the hydrodynamic equations, but they are similar to them. First we define the number density, n , and the momentum density (divided by the particle mass m), $n\mathbf{u}$,

where \mathbf{u} is the local average velocity. The pressure tensor (divided by m) is P_{ij} , and the kinetic energy density (divided by m) is ne_k ; they are all defined in terms of the local distribution function $f(\mathbf{r}, \mathbf{v}, t)$. The spatial and time coordinates are understood implicitly.

$$n = \int f(\mathbf{v}) d\mathbf{v} \quad (4)$$

$$n\mathbf{u} = \int \mathbf{v} f(\mathbf{v}) d\mathbf{v} \quad (5)$$

$$\begin{aligned} nP_{ij} &= \int f(\mathbf{v})(\mathbf{v} - \mathbf{u})_i(\mathbf{v} - \mathbf{u})_j d\mathbf{v} \\ &= \int f(\mathbf{v})(\mathbf{c})_i(\mathbf{c})_j d\mathbf{c} = \int f(\mathbf{v})c_i c_j d\mathbf{c} \end{aligned} \quad (6)$$

$$ne_k = 1/2 \int f(\mathbf{v})|\mathbf{v}|^2 d\mathbf{v} \quad (7)$$

Here \mathbf{u} is the average (or macroscopic) velocity and \mathbf{c} is relative velocity

$$\mathbf{c} = \mathbf{v} - \mathbf{u} \quad (8)$$

We also define the heat flux vector (that include both the convective and the diffusive heat flux)

$$\mathbf{q} = 1/2 \int f(\mathbf{v})|\mathbf{v}|^2 \mathbf{v} d\mathbf{v} \quad (9)$$

The three collisional invariants are $\psi(\mathbf{v}) = 1$, \mathbf{v} and $|\mathbf{v}|^2/2$. They express the local conservation of matter, momentum and energy. Using them in Eq. (3) we get the conservation equations for the space and time dependence of the local number density, the local velocity and the local kinetic energy. Here \otimes denotes the tensor product.

$$\frac{\partial n}{\partial t} + \nabla_x \cdot n\mathbf{u} = 0 \quad (10)$$

$$\frac{\partial n\mathbf{u}}{\partial t} + \nabla_x \cdot n(\mathbf{u} \otimes \mathbf{u} + \mathbf{P}) = n\mathbf{F} \quad (11)$$

$$\frac{\partial ne_k}{\partial t} + \nabla_x \cdot \mathbf{q} = n\mathbf{F} \cdot \mathbf{u} \quad (12)$$

In component notation they are

$$\frac{\partial n}{\partial t} + \frac{\partial nu_j}{\partial x_j} = 0 \quad (13)$$

$$\frac{\partial nu_i}{\partial t} + \frac{\partial}{\partial x_j} [n(u_i u_j + P_{ij})] = n\mathbf{F}_i \quad (14)$$

$$\frac{\partial ne_k}{\partial t} + \frac{\partial \mathbf{q}_j}{\partial x_j} = n\mathbf{F}_j u_j \quad (15)$$

The Euler equations of hydrodynamics can be obtained from Eq. (13) - (15) by multiplying them by the mass of a particle, m , using $\rho = nm$ and adding in the internal energy, ϵ_{mat} , and the specific enthalpy or heat function w , of the matter.

$$\frac{\partial \rho}{\partial t} + \nabla_x \cdot \rho \mathbf{u} = 0 \quad (16)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = \rho \mathbf{F} \quad (17)$$

$$\frac{\partial}{\partial t} (\epsilon_{mat} + \frac{1}{2} \rho u^2) + \nabla \cdot (\rho \mathbf{u} w + \frac{1}{2} \rho \mathbf{u} u^2) = \rho \mathbf{F} \cdot \mathbf{u} \quad (18)$$

The hydrodynamic equations are written for a continuum and they are valid only on much longer spatial scales and time scales than the collisions. The Navier - Stokes equations have added viscosity terms. In addition, there are fluctuations in fluids that are not described by the Navier - Stokes equations. The difficulty in establishing the hydrodynamic limit of the Boltzmann equations stems from the fact that in order to calculate the stress tensor, $p = mP$ and the viscosity, one has to “close” the Boltzmann equation hierarchy. The traditional way of doing this is an expansion in terms of the (small) ratio of the collision range, $l = (1/n)^{1/3}$, to the length, L , of the reciprocals of the typical gradients. This is the Knudsen number, $\text{Kn} = l/L$.

At this point we want to discuss entropy generation, i.e. Boltzmann’s H theorem. We refer to Villani’s treatise [6]. The collision operator, $Q(f, f)$, for energy and momentum conserving collisions has the form

$$Q(f, f) = \int d\mathbf{v}_* \int d\sigma B(\mathbf{v} - \mathbf{v}_*, \sigma) (f' f'_* - f f_*) \quad (19)$$

In this equation \mathbf{v}, \mathbf{v}_* are the incoming particle velocities, and $\mathbf{v}', \mathbf{v}'_*$ are the outgoing particle velocities and similarly f, f_* and f', f'_* are the incoming and outgoing particle distributions respectively. The angular deviation of the relative velocities on a collision is σ .

The notation in this equation is somewhat opaque. For later use and for some clarity we will write down a more general collision operator, similar to Eq. (3), but valid for the collisions of two different species. We define the binary collision operator as

$$Q(g_b, f_a) = \int d\mathbf{v}_b \int d\sigma B(n_a \mathbf{v}_a - n_b \mathbf{v}_b, \sigma) (g'_b f'_a - g_b f_a) \quad (20)$$

Here a, b are two species of colliders, n_a, n_b can be thought of as their masses expressed as number densities. The expression $Q(g_b, f_a)$ is the rate of change of an a particle by collisions with all b particles having the velocity distribution g_b . In the collision the a particle has a momentum $n_a \mathbf{v}_a$. It collides with a b particle of momentum $n_b \mathbf{v}_b$ and the momentum difference is rotated by σ , that is a momentum transfer vector. Because collisions conserve the number of particles as well as total momentum and energy, the vector σ uniquely defines the outgoing momenta $n_a \mathbf{v}'_a, n_b \mathbf{v}'_b$. The collisions result in a loss for $f_a(\mathbf{v}_a)$, so they contribute a negative term. The positive term comes from the reverse collisions, where particles with the outgoing momenta collide to produce particles with the original momenta. By the reversibility of the equations of motion, they have the same probability. The inner integral is over the momentum transfer, σ and the outer integral is over all the possible velocities of the collider, \mathbf{v}_b .

The Boltzmann H function, the negative of the entropy of the distribution, is

$$H(f) = \int d\mathbf{v} f \log f \quad (21)$$

As f evolves, H decreases in time (the entropy of the distribution increases in time.) The dissipation rate of H is given by

$$d(f) = \frac{1}{4} \int d\mathbf{v} d\mathbf{v}_* d\sigma B(\mathbf{v} - \mathbf{v}_*, \sigma) (f' f'_* - f f_*) \log \frac{f' f'_*}{f f_*} \geq 0 \quad (22)$$

An important corollary is that the dissipation of H vanishes *if and only if* the distribution is the “local” Maxwell - Boltzmann distribution,

$$M(\mathbf{c}) = \frac{n}{(2\pi RT)^{3/2}} \exp\left(-\frac{|\mathbf{c}|^2}{2RT}\right) \quad (23)$$

Here $R = k/m$ and n , as well as RT , are space and time dependent. Explicitly, $M \equiv M(\mathbf{r}, \mathbf{c}, t; n, \mathbf{u}, RT)$.

3 The Boltzmann equation in the difference form

The next step has its motivation in the work of Szoke and Brooks [1] on radiation transport. It was observed that in optically thick media (far from boundaries and transients), the radiation is close to thermal. In other words, the emission and absorption of radiation are two large quantities that almost cancel each other while their difference is comparatively small. Following this hint, the radiation intensity was decomposed into a sum of the local black body (Planckian) distribution and a (space, frequency, and time-dependent) local deviation from it. When the radiation intensity is written as a sum of the local Planckian and the deviation field, the propagation operator in the transport equation acts on the deviation field alone, while the space-time variation of the local Planckian becomes the source of the deviation field. As the deviation of the local intensity from the Planckian becomes small in thick media far from boundaries, modeling the difference field has obvious advantages for Monte Carlo calculations. We called the result the “difference formulation” of radiation transport.

Similarly, in regimes where collisions dominate and where gradients of the parameters are small, the distribution function, $f(\mathbf{r}, \mathbf{v}, t)$, gets close to a Maxwellian. This is the hydrodynamic regime. Although the collisions are the dominant term, “forward” and “reverse” collisions almost cancel and their net effect becomes small. As in radiation transport, the spatial and temporal changes in the local Maxwell distribution become the source of the deviations of $f(\mathbf{r}, \mathbf{v}, t)$ from a Maxwellian and they are the terms that contribute to the transport of particles, momentum and energy.

The rest of the paper is devoted to the development and discussion of this picture. We formally decompose the distribution function f into a local Maxwellian and a difference velocity distribution

$$f = M + D \tag{24}$$

The variables are to be understood.

Substituting into Eq. (1), we get the “difference Boltzmann equation”

$$\begin{aligned} \frac{\partial D}{\partial t} + \mathbf{v} \cdot \nabla_x D + \mathbf{F} \cdot \nabla_v D &= Q(M, D) + Q(D, M) + Q(D, D) \\ &\quad - \frac{\partial M}{\partial t} - \mathbf{v} \cdot \nabla_x M - \mathbf{F} \cdot \nabla_v M. \end{aligned} \tag{25}$$

Note that $Q(M, M) = 0$.

This innocuous looking transformation is the main innovation in our approach. It introduces a new point of view. The derivatives of the local Maxwell distributions are the sources of the difference distribution, *i.e.* the deviation of the distribution from Maxwellian. These gradients are the deviations from global equilibrium. So, in global equilibrium the difference field vanishes. The left hand side of the equation and the collision terms describe the evolution of the difference field.

Six remarks are in order. First, the decomposition is *exact*, it is not perturbative. An important new property of the difference distribution, D , is that it can have positive and negative parts, while f is always non-negative. From the non-negativity of f it follows that D is bounded from below, $D \geq -f$ for all velocities and everywhere. The D particles are true “negative particles”: they have negative mass, negative energy and they carry negative momentum. The connection with perturbation theory is that choosing a “good” set of parameters for M , makes D “small”. Second, the derivative terms on the right hand side are the sources for the difference density. They are very similar to the “new” sources in the difference formulation of radiation transport [1]. Third, in the relaxation approximation (that should be used very sparingly - as we will show below) our difference equation (25) is identical to the difference equations of radiative transport. The main difference between the Boltzmann equation and the radiation transport equation is that photons are *not* conserved but particles are. Fourth, if the Knudsen number is small, $\text{Kn} = \epsilon \ll 1$, we expect that $Q(M, D) \approx \epsilon$ and $Q(D, D) \approx \epsilon^2$. Fifth, we note that the approach to local equilibrium is dominated by the $Q(M, D)$ term. To calculate the steady state fluctuations the $Q(D, D)$ term has to be included. Sixth, the source terms have a tensorial character in velocity. As M has an angular distribution of the spherical harmonic P_0 , the sources for D are at most P_2 . This fact has important implications. A generalization that works in radiation transport is to use a more general “reference field”. As long as the reference field has a P_0 character in velocity, the sources for D are still at most of P_2 character in velocity.

At this point the Maxwellian can have an arbitrary set of parameters. Note from Eq. (23) that the distribution is characterized by five parameters: n , \mathbf{u} and RT . As mentioned above, one of the central tasks will be to find “optimal” values of these parameters in order to minimize D in some sense. In fact, the equations for the conservation of mass, momentum, and energy determine the evolution of those parameters in space and time. The result will be a set of equations for the parameters that lead to generalizations of the Euler equations above.

Equation (25) has the general form

$$\frac{dD}{dt} = \left. \frac{dD}{dt} \right|_{coll} + \left. \frac{dD}{dt} \right|_{source}. \quad (26)$$

The constraint of non-negativity on f demands that the particles emitted by the sources can not be more negative than the local Maxwellian at any velocity. We also note that if D emitted by the sources does satisfy the positivity constraint, $(M + D) \geq 0$, during its propagation the same sources add the right amount to it that $M + D$ stays non-negative.

We will now develop the equations for the sources and the propagation of D ; then we develop the collision operators $Q(M, D)$; and then we write down the conservation equations that D has to satisfy. The set of six equations are needed for the solution of an initial value problem.

3.1 The sources and propagation of D

The next step is to calculate explicitly the three “new” source terms on the right hand side of Eq. (25), using the chain rule of differentiation. In the similar derivation in radiation transport, the only parameter in the Planckian is the temperature, that varies in space and time. In hydrodynamics $M(\mathbf{r}, \mathbf{c}, t; n, \mathbf{u}, RT)$ depends on n, \mathbf{u}, RT ; i.e. the local density, average velocity and temperature in energy units, all of which vary in space and time.

We will display the individual terms. As previously, we use $\mathbf{v} - \mathbf{u} = \mathbf{c}$

$$\begin{aligned} \frac{\partial M}{\partial t} &= \frac{\partial M}{\partial n} \frac{\partial n}{\partial t} + \dots = \\ M \left[\frac{1}{n} \frac{\partial n}{\partial t} + \frac{1}{RT} (c_j \frac{\partial u_j}{\partial t}) + \left(-\frac{3}{2} + \frac{|\mathbf{c}|^2}{2RT} \right) \frac{1}{RT} \frac{\partial RT}{\partial t} \right] \end{aligned} \quad (27)$$

$$\begin{aligned} \mathbf{v} \cdot \nabla_x M &= v_j \frac{\partial M}{\partial x_j} = \\ M \left[v_j \frac{1}{n} \frac{\partial n}{\partial x_j} + v_j \frac{1}{RT} (c_i \frac{\partial u_i}{\partial x_j}) + v_j \left(-\frac{3}{2} + \frac{|\mathbf{c}|^2}{2RT} \right) \frac{1}{RT} \frac{\partial RT}{\partial x_j} \right] \end{aligned} \quad (28)$$

$$\mathbf{F} \cdot \nabla_v M = -\mathbf{F} \cdot \nabla_u M = -M \mathbf{F} \cdot \frac{\mathbf{c}}{RT} = -M \mathbf{F}_j \frac{c_j}{RT} \quad (29)$$

Collecting all the terms, we get

$$\begin{aligned}
\frac{\partial D}{\partial t} + \mathbf{v} \cdot \nabla_x D + \mathbf{F} \cdot \nabla_v D - Q(M, D) - Q(D, M) - Q(D, D) = \\
-M \left[\frac{1}{n} \frac{\partial n}{\partial t} + \frac{1}{RT} (c_j \frac{\partial u_j}{\partial t}) + (-\frac{3}{2} + \frac{|\mathbf{c}|^2}{2RT}) \frac{1}{RT} \frac{\partial RT}{\partial t} \right. \\
+ v_j \frac{1}{n} \frac{\partial n}{\partial x_j} + v_j \frac{1}{RT} (c_i \frac{\partial u_i}{\partial x_j}) + v_j (-\frac{3}{2} + \frac{|\mathbf{c}|^2}{2RT}) \frac{1}{RT} \frac{\partial RT}{\partial x_j} \\
\left. - \mathbf{F}_j \frac{c_j}{RT} \right] \quad (30)
\end{aligned}$$

The sources of the difference field have three forms of velocity dependence: M , $\mathbf{c}M$ and $|\mathbf{c}|^2 M$. They can be positive or negative, depending on the relative magnitudes and signs of the time- and space-derivatives. Also, the collision terms, $-Q(M, D) - Q(D, M) - Q(D, D)$ always relax the difference field *and they conserve the particle number, the momentum and the energy*. (The situation is similar in the difference formulation of radiation transport. There energy and momentum are conserved, but photons appear and disappear at will, and they also don't collide with each other.) We glossed over the added condition, that for all velocities $M + D \geq 0$. This can be a serious difficulty for mathematical analysis as well as for real problems.

3.2 Collision operators and collisional invariants

In order to determine the evolution of the parameters of M we have to integrate Eq. (25) in the difference formulation, using the collision operators and the collisional invariants. The integrals are far from trivial. This produces a new version of the hydrodynamic equations and the deviations from them. This is very similar to the Chapman - Enskog expansion, but we expect that it is more transparent, non-perturbative, therefore more accurate and even more consistent. (From our experience with radiation transport, we hope that the orders of the expansion will not be mixed, *i.e.* the “closure” problem of the Chapman - Enskog expansion may be alleviated.)

The integrals to be evaluated are of the general form, from Eq. (1)

$$\begin{aligned}
\frac{\partial}{\partial t} \int \psi f d\mathbf{v} + \frac{\partial}{\partial x_j} \int \psi v_j f d\mathbf{v} + \mathbf{F}_j \int \psi \frac{\partial f}{\partial v_j} d\mathbf{v} \\
- \int \frac{\partial \psi}{\partial t} f d\mathbf{v} - \int \frac{\partial \psi}{\partial x_j} v_j f d\mathbf{v} = \int \psi Q(f, f) d\mathbf{v} \quad (31)
\end{aligned}$$

Here $f = M + D$. For the conservation of particles $\psi = 1$, for momentum conservation $\psi = v_i$ and for energy conservation $\psi = |\mathbf{v}|^2/2$.

As $\mathbf{v} = \mathbf{u} + \mathbf{c}$ and \mathbf{u} is constant at every point in space, we will change the variable of integration to \mathbf{c} .

3.2.1 The number density

First we note that the correct particle density is *not* the one that appears in M in Eq. (23). In fact, some of the source terms in Eq. (30), that are proportional to $\partial n / \partial t$ and $\partial T / \partial t$, give a non-zero density for D .

We will now evaluate Eq. (31) with $\psi = 1$.

First some definitions. We decompose D into a symmetric and antisymmetric part

$$D_{sym} = (1/2)(D(\mathbf{c}) + D(-\mathbf{c})) \quad (32)$$

$$D_{as} = (1/2)(D(\mathbf{c}) - D(-\mathbf{c})) \quad (33)$$

We also note that M is symmetric. An interesting property of both M and D_{sym} is that they contribute to the density and the energy, but they have no net momentum in the comoving system, where $\mathbf{u} = 0$. In the same system D_{as} contributes no density, no energy but does have a net momentum.

We define

$$n_M = \int M d\mathbf{c} \quad (34)$$

$$n_D = \int D_{sym} d\mathbf{c} \quad (35)$$

By symmetry,

$$\int D_{as} d\mathbf{c} = 0 \quad (36)$$

We calculate now the individual terms

$$\int \frac{\partial}{\partial t} (M + D) d\mathbf{c} = \frac{\partial}{\partial t} \int (M + D_{sym}) d\mathbf{c} = \frac{\partial}{\partial t} (n_M + n_D) \quad (37)$$

$$\frac{\partial}{\partial x_j} \int (u_j + c_j)(M + D) d\mathbf{c} = \frac{\partial}{\partial x_j} \left[u_j (n_M + n_D) + \int c_j D_{as} d\mathbf{c} \right] \quad (38)$$

This result needs some clarification: The difference density is $D = D_{sym} + D_{as}$.

The integral $\int c_j D_{sym} d\mathbf{c} = 0$ by symmetry. The integral

$$\int c_j D_{as} d\mathbf{c} = \int c_j D_{as} dc_i dc_j dc_k \quad (39)$$

is NOT necessarily zero.

The influence of the external force is (again in components)

$$F_j \int \frac{\partial}{\partial v_j} (M + D) d\mathbf{c} = F_j \int \frac{\partial}{\partial c_j} (M + D) d\mathbf{c} = 0 \quad (40)$$

The integrals over M and D_{sym} vanish by symmetry. The integral

$$\int \frac{\partial}{\partial c_j} D_{as} dc_j = D_{as}(+\infty) - D_{as}(-\infty) = 0 \quad (41)$$

The two last integrals on the left hand side of Eq. (31) are zero, because $\psi = 1$ is independent of x and t . As $\int d\mathbf{c}$ is a collisional invariant,

$$\int [-Q(M, D) - Q(D, M) - Q(D, D)] d\mathbf{c} = 0 \quad (42)$$

Our number density equation is, finally

$$\frac{\partial}{\partial t} (n_M + n_D) + \nabla_x \cdot \left[\mathbf{u} (n_M + n_D) + \int \mathbf{c} D_{as} d\mathbf{c} \right] = 0 \quad (43)$$

In component notation

$$\frac{\partial}{\partial t} (n_M + n_D) + \frac{\partial}{\partial x_j} \left[u_j (n_M + n_D) + \int c_j D_{as} d\mathbf{c} \right] = 0 \quad (44)$$

3.2.2 Momentum conservation

We will now evaluate Eq. (31) with $\psi = v_i$. Again we will display the individual terms.

$$\frac{\partial}{\partial t} \int v_i (M + D) d\mathbf{c} = \frac{\partial}{\partial t} u_i (n_M + n_D) \quad (45)$$

This is the definition of the mean velocity, u_i . It can be shown that it is compatible with all our previous definitions. (In fact, in Eq. (41) we have shown the detailed argument.)

$$\begin{aligned}
& \frac{\partial}{\partial x_j} \int (u_i + c_i)(u_j + c_j)(M + D)d\mathbf{c} = \\
& \frac{\partial}{\partial x_j} \left[u_i u_j (n_M + n_D) + u_i \int c_j D_{as} d\mathbf{c} + u_j \int c_i D_{as} d\mathbf{c} + \right. \\
& \quad \left. \int c_i c_j (M + D) d\mathbf{c} \right]
\end{aligned} \tag{46}$$

The last integral is the stress tensor,

$$P_{ij} = \int c_i c_j (M + D) d\mathbf{c} = P_{ijM} + P_{ijD} \tag{47}$$

$$\begin{aligned}
F_j \int v_i \frac{\partial}{\partial v_j} (M + D) d\mathbf{c} &= F_j \int \frac{\partial}{\partial v_j} [v_i (M + D)] d\mathbf{c} - \\
& F_j \int \frac{\partial v_i}{\partial v_j} (M + D) d\mathbf{c} = 0 - \delta_{ij} F_j (n_M + n_D)
\end{aligned} \tag{48}$$

The two last integrals on the left hand side of Eq. (31) are zero, because $\psi = v_i$ is independent of x and t . This is not an obvious fact, but the definition of v_i is just a “quantity”. As a collisional invariant, the collision integral is zero:

$$\int v_i [-Q(M, D) - Q(D, M) - Q(D, D)] d\mathbf{c} = 0. \tag{49}$$

Finally, the momentum balance equation is

$$\begin{aligned}
& \frac{\partial}{\partial t} u_i (n_M + n_D) + \frac{\partial}{\partial x_j} \left[u_i u_j (n_M + n_D) + \right. \\
& \left. u_i \int c_j D_{as} d\mathbf{c} + u_j \int c_i D_{as} d\mathbf{c} + (P_{ijM} + P_{ijD}) \right] = F_i (n_M + n_D)
\end{aligned} \tag{50}$$

3.2.3 Energy conservation

We will now evaluate Eq. (31) with $\psi = |\mathbf{v}|^2/2 = (v_i v_i)/2$. Again we will display the individual terms.

$$\begin{aligned}
\frac{1}{2} \frac{\partial}{\partial t} \int v_i v_i (M + D) d\mathbf{c} &= \frac{1}{2} \frac{\partial}{\partial t} u_i u_i \int (M + D) d\mathbf{c} + \\
& \frac{\partial}{\partial t} u_i \int c_i (M + D) d\mathbf{c} + \frac{1}{2} \frac{\partial}{\partial t} \int c_i c_i (M + D) d\mathbf{c} = \\
& \frac{\partial}{\partial t} \left[\frac{|\mathbf{u}|^2}{2} + \epsilon_{int} \right] (n_M + n_D)
\end{aligned} \tag{51}$$

Here the “internal” kinetic energy was defined as

$$\epsilon_{int}(n_M + n_D) = \frac{1}{2} \int c_i c_i (M + D) d\mathbf{c} \quad (52)$$

The next term in Eq. (31) is

$$\frac{1}{2} \frac{\partial}{\partial x_j} \int (u_i + c_i)(u_i + c_i)(u_j + c_j)(M + D) d\mathbf{c} \quad (53)$$

It is a sum of six terms. We will display them individually. The first one is the transport of translational kinetic energy,

$$\frac{1}{2} \frac{\partial}{\partial x_j} u_j u_i u_i \int (M + D) d\mathbf{c} = \frac{\partial}{\partial x_j} u_j (|\mathbf{u}|^2/2)(n_M + n_D) \quad (54)$$

The three terms with $u^2 c$ are

$$\frac{1}{2} u_i u_i \int c_j D_{as} d\mathbf{c} + u_i u_j \int c_i D_{as} d\mathbf{c} \quad (55)$$

$$\frac{1}{2} \frac{\partial}{\partial x_j} u_j \int c_i c_i (M + D) d\mathbf{c} = \frac{\partial}{\partial x_j} u_j \epsilon_{kin}(n_M + n_D) \quad (56)$$

The next two terms are

$$\frac{1}{2} \frac{\partial}{\partial x_j} u_i \int c_i c_j (M + D) d\mathbf{c} = \frac{1}{2} \frac{\partial}{\partial x_j} u_j (P_{jiM} + P_{jiD}) \quad (57)$$

The fourth term is

$$\begin{aligned} & \frac{1}{2} \frac{\partial}{\partial x_j} \int c_i c_i c_j (M + D) d\mathbf{c} = \\ & \frac{1}{2} \frac{\partial}{\partial x_j} \int c_i c_i c_j D_{as} d\mathbf{c} = \frac{1}{2} \frac{\partial}{\partial x_j} P_{ijD} = \frac{\partial}{\partial x_j} \mathbf{q}_j \end{aligned} \quad (58)$$

The integrals over M and D_{sym} are zero by symmetry. This equation also defines the diffusive heat flux vector \mathbf{q} .

The external force term is

$$\begin{aligned} & F_j \frac{1}{2} \int (u_i + c_i)(u_i + c_i) \frac{\partial}{\partial v_j} (M + D) d\mathbf{c} = \\ & 0 - F_j \frac{1}{2} 2u_i \int c_i \frac{\partial}{\partial c_j} (M + D) d\mathbf{c} + 0 = -F_j u_j (n_M + n_D) \end{aligned} \quad (59)$$

The last two terms and the collision terms integrate to zero.

So, finally the energy conservation equation is

$$\begin{aligned} & \frac{\partial}{\partial t} \left[\frac{|\mathbf{u}|^2}{2} + \epsilon_{int} \right] (n_M + n_D) + \\ & \frac{\partial}{\partial x_j} \left[u_j \left(\frac{|\mathbf{u}|^2}{2} + \epsilon_{int} \right) (n_M + n_D) + \frac{1}{2} u_i u_i \int c_j D_{as} d\mathbf{c} + \right. \\ & \quad \left. u_i u_j \int c_i D_{as} d\mathbf{c} + \frac{1}{2} P_{ijD} \right] = F_j u_j (n_M + n_D) \end{aligned} \quad (60)$$

The main conclusion is that these equations are very similar to the ones obtained from a straightforward evaluation of a general f but they are not identical to them.

3.3 Summary

In summary, the set of three conservation equations, (44), (50), (60) have to be solved together with the propagation equation for D , Eq. (30). One way to perceive them is as an initial value problem. In this view we can assign an arbitrary set of values for the parameters of the Maxwellian, $M(\mathbf{r}, \mathbf{c}, t; n, \mathbf{u}, RT)$, and follow the evolution of the parameters in space and time.

This includes the possibility to assign initially $n = 0$ everywhere; that reduces our difference equations to the original Boltzmann equation and “no harm has been done”.

4 The hydrodynamic limit: Navier - Stokes equations and beyond

As discussed in the previous subsection, in principle we can start with an arbitrary distribution of Maxwellians in space at a given time and let their parameters evolve according to the four equations: the propagation equation for D , Eq. (30), the conservation equations for the number of particles, for the momentum and for the energy, Eqs. (44), (50), (60). The last three equations are similar to the equations of hydrodynamics, but there are no approximations in their derivation. It is interesting to investigate their “hydrodynamic limit”, *i.e.* how they relate to the compressible Navier - Stokes equations.

In hydrodynamics the equation of state plus the three Euler equations, (13), (14), (15) govern the space and time dependence of the density of the fluid,

of its momentum density and of its energy density (or temperature), ρ, \mathbf{u}, RT . In the Boltzmann equation those are the parameters of the local equilibrium (Maxwellian) distribution function, $M(\mathbf{r}, \mathbf{c}, t; n, \mathbf{u}, RT)$; but in the hydrodynamic description there is no mention of the velocity distribution function of the particles. The development of the distribution $f(\mathbf{r}, \mathbf{v}, t)$ in time involves an additional equation, the original Boltzmann equation, (2). In the traditional Chapman - Enskog, or Hilbert expansion the distribution function, f , is somehow assumed to be a local equilibrium distribution, $M(\mathbf{r}, \mathbf{c}, t; n, \mathbf{u}, RT)$ but it is not “really” so; otherwise there would be no diffusive transport and all the richness of non - equilibrium phenomena in gases would be lost. *Our modest contribution is to make the deviation of f from a local Maxwellian explicit and write the evolution equations for the hydrodynamic variables, n, \mathbf{u}, RT , as explicit functions of this deviation, D .*

We now start from the other end and discuss the equations of hydrodynamics. The standard way to get the compressible Navier - Stokes equations, in Landau - Lifshitz's notation, is to *add* linear viscosity and linear heat conduction (diffusion) to the Euler equations [10]. We will write those equations in component notation.

The Navier - Stokes equation for the conservation of matter, without body forces, is

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \quad (61)$$

The momentum conservation equation is

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j} [\rho(u_i u_j + P_{ij})] = \frac{\partial}{\partial x_j} \sigma'_{ij} \quad (62)$$

Here a viscous stress (or transport) term was added. It is

$$\sigma'_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right) + \zeta \left(\delta_{ij} \frac{\partial u_l}{\partial x_l} \right) \quad (63)$$

μ is the shear viscosity and ζ is the volume viscosity.

The equation for the energy also has two terms added,

$$\frac{\partial}{\partial t} \left(\frac{1}{2} \rho u^2 + \epsilon_{mat} \right) + \frac{\partial}{\partial x_j} \left[\rho u_j \left(\frac{1}{2} \rho u^2 + w \right) - u_i \sigma'_{ij} - \kappa \frac{\partial T}{\partial x_j} \right] = 0 \quad (64)$$

κ is the thermal conduction. We remind the reader that ϵ_{mat} is the internal energy and w is the heat function (enthalpy) of the matter.

We can now compare these equations to the conservation equations in the difference formulation, Eqs. (44), (50), (60).

The equations for the density Eqs. (44), (61) are very similar. The total density is $\rho = m(n_M + n_D)$. In the Boltzmann (difference) formulation there is an additional term

$$\frac{\partial}{\partial x_j} \int c_j D_{as} d\mathbf{c}. \quad (65)$$

The additional term expresses the fact that a space varying antisymmetric difference density does contribute to the density of particles.

We now compare the momentum conservation equations Eqs. (50), (62), using $P_{ij} = (P_{ijM} + P_{ijD})$. The terms corresponding to the viscous stress tensor, in the Boltzmann formulation, are

$$\frac{\partial}{\partial x_j} \left[u_i \int c_j D_{as} d\mathbf{c} + u_j \int c_i D_{as} d\mathbf{c} \right] \equiv -\frac{\partial}{\partial x_j} \sigma'_{ij} \quad (66)$$

Again this is a pleasing result, it shows that in the linear regime the viscosity is proportional to the velocity gradient tensor.

Finally, we compare the energy conservation equations, Eqs. (60), (64). They are again very similar, but their differences need some discussion.

First, there is an equivalence between our notation and the notation of Landau Lifshitz in the Navier Stokes equation, [10]: our $n\epsilon_{kin}$ corresponds to L-L's ϵ_{mat} in the time dependent term and to w in the heat flux term. We ignore these differences. The equivalence is then

$$\frac{\partial}{\partial x_j} \left[\frac{1}{2} u_i u_i \int c_j D_{as} d\mathbf{c} + u_i u_j \int c_i D_{as} d\mathbf{c} + \frac{1}{2} P_{iijD} \right] \equiv -\frac{\partial}{\partial x_j} \left[u_i \sigma'_{ij} + \kappa \frac{\partial T}{\partial x_j} \right] \quad (67)$$

Again this is a pleasing result. Considering Eq. (66), there is an equivalence between $(1/2)P_{iijD}$ and $-\kappa(\partial T/\partial x_j)$. In Eq. (58) we identified the diffusive heat flux, \mathbf{q}_j with $(1/2)P_{iijD}$, so our equivalence affirms the first order expansion of the diffusive heat flux being proportional to the negative of the temperature gradient.

Our results show that the Navier Stokes equations of hydrodynamics are indeed the first approximation to the solution of the Boltzmann equation together with the conservation equations. We think that our derivation, that has no approximations, is much more transparent than the Hilbert, or the Chapman - Enskog expansions. In addition, it is a very simple recipe to get

viscosity and heat conductivity to any order. Also, it shows that dilute gases have no “hidden” properties in any regime.

5 Simple applications

In order to show the utility of our approach we calculate a transport coefficient: the thermal conductivity. We will also comment on the limitations of our derivation and on the lowest order non - linear modification of the thermal conductivity.

Then we will attempt to calculate a simple boundary layer, then a shock structure in a dilute gas...?

5.1 The thermal conductivity

From Eq. (30) it follows that the difference distribution produced by a density and/or temperature gradient is always a P_1 distribution with an axis along the direction of the gradients of the temperature and the density. (If the two gradients point in different directions, the distribution can be of a net P_2 character.) If the gradients point in the same direction, D has a zero net particle number, a zero net energy *but a finite momentum*. The latter is the source of many of the difficulties in the solution of the equations.

In order to wet our feet, (whet our appetite?) we will investigate the following steady state problem.

A finite slab of a dilute gas has a thermal gradient and an opposing density gradient imposed on it. There is no external force. We can imagine that the slab is finite in the x direction and infinite in the y, z directions. We also demand that the pressure be constant in the slab and that it has relaxed to its steady state, so nothing is time dependent. There is no mean velocity anywhere, but the temperature gradient is maintained externally. The thermal conductivity is the ratio of the diffusive thermal flux and the (negative of) temperature gradient.

Considering the propagation equation for the difference density, Eq. (30), the only terms left are

$$\frac{\partial D}{\partial t} + \mathbf{c} \cdot \nabla_x D - Q(M, D) - Q(D, M) - Q(D, D) =$$

$$-M \left[c_x \frac{1}{n} \frac{dn}{dx} + c_x \left(-\frac{3}{2} + \frac{|\mathbf{c}|^2}{2RT} \right) \frac{1}{RT} \frac{dRT}{dx} \right] \quad (68)$$

The sources of D have a P_1 type distribution in the local velocity, with its axis in the direction of c_x , the direction of the gradient. The dependences of the sources on $|\mathbf{c}|$ are different for the two gradients. The density gradient source is positive in the direction of the lower density, and negative in the direction of the higher density for all velocities. The temperature gradient source is more complicated: it is as expected at high velocities, $|\mathbf{c}|^2 > 3RT$, but it is reversed at low velocities. The angular distribution is still P_1 , but the positive lobe is in the direction of the higher temperature at low velocities. This behavior is “reasonable”, considering that a Maxwell distribution with a given number of particles is broader at higher temperatures and has a lower peak at lower velocities.

The number and energy conservation equations, (44), (60) are satisfied identically. The momentum conservation equation, (50), reduces to

$$\frac{\partial}{\partial x} (P_{ijM} + P_{ijD}) = \frac{1}{2} \frac{\partial}{\partial x} \int c_x c_x (M + D) d\mathbf{c} = 0 \quad (69)$$

All the terms that contain \mathbf{u} are zero, so is the time derivative. As D is antisymmetric in c_x , the second term in the integral is also zero.

The calculation is straightforward. (For completeness, it will be presented below.) The result is

$$\frac{1}{n} \frac{dn}{dx} = -\frac{1}{RT} \frac{dRT}{dx} \quad (70)$$

This shows that the Boltzmann equation has the equation of state of an ideal gas, and that in our example the pressure is constant, so for an ideal gas $nRT = p = \text{const.}$

Equation (68) then simplifies to

$$\begin{aligned} \frac{\partial D}{\partial t} + \mathbf{c} \cdot \nabla_x D - Q(M, D) - Q(D, M) - Q(D, D) = \\ -nM_1 c_x \left(-\frac{5}{2} + \frac{|\mathbf{c}|^2}{2RT} \right) \frac{1}{RT} \frac{dRT}{dx_j}, \end{aligned} \quad (71)$$

where we defined the unit Maxwell distribution

$$M_1(\mathbf{c}) = \frac{M(\mathbf{c})}{n} = \frac{1}{(2\pi RT)^{3/2}} \exp\left(-\frac{|\mathbf{c}|^2}{2RT}\right) \quad (72)$$

Eq. (71) is the same as used by Kremer [9] (Eq. 34), and Landau [8] (Eq. 10.1). In particular, $5/2$ is the constant pressure heat capacity, c_p .

The right hand side of Eq. (71) is the source of D , while the left hand side is the propagation of D and its relaxation by collisions. It is the collision integral that traditionally causes all the difficulties. We will approximate the collisions by a relaxation that conserves the particle number, the momentum and the energy.

In order to calculate the diffusive heat flux, we have to calculate the difference field D . As a preliminary consideration, we consider a point in space, \mathbf{x} and a difference particle emitted with velocity \mathbf{c} at a time t . We will denote this difference field by $D(\mathbf{x}, t; c, \Omega)$.¹ In our case, where the distribution of D has an angular dependence of P_1 (with its axis in the x direction) it is advantageous to consider pairs of particles, that are emitted in opposite directions with velocities \mathbf{c} , $-\mathbf{c}$. Their total particle number and energy are zero, but their net momentum is non-zero. When the pair is emitted, the Maxwellian source recoils, in order to conserve momentum. As they propagate they relax into the local Maxwellian and they deposit their momentum into it. By choosing the relation (70) between dn/dx and dRT/dx we guarantee that the momentum of the emission (and the absorption), integrated over the velocity is zero everywhere, so the momentum conservation equation is satisfied.

The collision term in the Boltzmann equation, in the most general case, is very difficult to calculate [6]. Here we will use a very simple version of the collision term: it is a relaxation using a mean free path, d along the direction of propagation of $D(\mathbf{c})$. (A better assumption would be that d is a function of velocity $d(|\mathbf{c}|)$.²) Such an approximation ignores the angular distribution of the collision kernel, it implicitly assumes that a collision “absorbs”, or “thermalizes” the incident particle. As discussed above, in our particular case such relaxation satisfies all the conservation equations.

We will make one further approximation, that the gradients are so small that in the sources we can approximate the Maxwellian in Eq. (71) with a constant temperature and density. We will remark on the non - linear extension of our calculation, when this approximation is not taken.

We start with a simple calculation. Assume that D propagates in a straight line, without attenuation. Let us concentrate on a point \mathbf{x} in space and on a time t . The emission of D in a volume ΔV over a time Δt is $[dD(\mathbf{x}, t)/dt]\Delta V \Delta t$, where we denoted the right hand side of Eq. (71) by $[dD(\mathbf{x}, t)/dt]$. When this

¹ This notation is slightly different from the notation for $M \equiv M(\mathbf{r}, \mathbf{c}, t; n, \mathbf{u}, RT)$.

² Note that the BGK relaxation, that uses a single relaxation time corresponds to a cross section that is proportional to $1/c$ and it is not conservative.

source propagates to $\mathbf{x} = 0$, $t = 0$ it gives a *partial* difference density

$$D(0, 0; c, \mathbf{\Omega}) = \frac{dD(\mathbf{x}, t)}{dt} \Delta V \Delta t \frac{1}{4\pi r^2} \quad (73)$$

We denoted $r^2 = |\mathbf{x}^2|$, for convenience. The source propagates in straight line, with velocity $c > 0$ in the direction of $\mathbf{\Omega}$. There are constraints on the emission volume and the emission time determined by c . The emission volume is a spherical shell of width Δr and area $r^2 d\mathbf{\Omega}$. As the particles propagate with velocity c , $\Delta r = c\Delta t$. For simplicity we did not write out the time constraint explicitly, but will take it into account in the following.

In order to get the total difference density, we have to integrate the sources over the full volume, taking into account the constraints. the integrals are

$$D(0, 0; c, \mathbf{\Omega}) = \int \frac{dD(r, -r/c)}{dt} \frac{1}{4\pi r^2} r^2 \frac{dr}{c} d\mathbf{\Omega} \quad (74)$$

In our simple approximation the source decays exponentially with its path proportionally to $n\sigma$ and σ is a cross section. This modifies the previous equation to

$$D(0, 0; c, \mathbf{\Omega}) = \int \frac{dD(r, -r/c)}{dt} \frac{1}{4\pi c} \exp\left(-\int_0^\infty n\sigma dr\right) d\mathbf{\Omega} \quad (75)$$

In our problem we approximate n as independent of space, Then that integral can be carried out and the result is

$$D(0, 0; c, \mathbf{\Omega}) = \frac{dD(r, -r/c)}{dt} \frac{1}{n\sigma c} \quad (76)$$

We note that in our simple example $dD(r, -r/c)/dt$ and n are independent of time and the integral $\int d\mathbf{\Omega}/4\pi = 1$.

From our derivation it is clear how to proceed when the source has time and space dependence. (The integrals get much nastier.) Our relaxation *Ansatz* does preserve the number of particles, the momentum and the energy for the derivative sources, but in reality the collision integrals are much more difficult. We do not know how to improve on this point.

We should repeat the additional limitations of our approach and some justifications for them. We essentially approximated only the $Q(M, D)$ collision term and neglected $Q(D, M) + Q(D, D)$. If $Q(M, D) \approx \epsilon$, so is $Q(D, M)$. The justification to neglect this term is that D is of P_1 symmetry and if we consider

the pair of particles with opposite velocities, their total particle number and energy are zero and the momentum they impart to the Maxwellian, if integrated over all velocities in the same direction, is also zero. So the net result should be a distortion of the Maxwellian by the collisions and that should relax quite rapidly. As discussed above, $Q(D, D) \approx \epsilon^2$. We also did not take into account that at all velocities $M + D \geq 0$. In our example it follows from the smallness of dRT/dx .

Putting together Eqs. (71) and (76) gives

$$D(0, 0; c, \mathbf{\Omega}) = -\frac{1}{n\sigma c} \frac{n}{RT} M_1 c_x \left(-\frac{5}{2} + \frac{|\mathbf{c}|^2}{2RT}\right) \frac{\partial RT}{\partial x} = -\frac{1}{\sigma RT} M_1 \cos \theta \left(-\frac{5}{2} + \frac{|\mathbf{c}|^2}{2RT}\right) \frac{\partial RT}{\partial x} \quad (77)$$

The diffusive kinetic energy flux is the same as \mathbf{q} in Eq. (9). We will write it in polar coordinates in \mathbf{c} space

$$F_{ke} = \mathbf{q} = \int_0^\infty c^2 dc \int_{-1}^1 d \cos \theta \left[D(0; c, \mathbf{\Omega}) \frac{c^2}{2} c \cos \theta \right] \quad (78)$$

The integral is straightforward. (For completeness, it will be presented below.) The result is

$$F_{ke} = -\frac{4}{3} \frac{1}{\sigma} \left(\frac{RT}{2\pi} \right)^{1/2} \frac{\partial RT}{\partial x} \quad (79)$$

5.1.1 Some integrals

We show now some details of the two integrals in Eqs. (69) and (78).

The momentum balance equation reduces to

$$\frac{1}{2} \frac{\partial}{\partial x} \int c_x c_x M d\mathbf{c} = \frac{1}{2} \int c_x c_x \frac{\partial M}{\partial x} d\mathbf{c} = 0 \quad (80)$$

From Eq. (28)

$$\frac{\partial M}{\partial x} = M \left[\frac{1}{n} \frac{\partial n}{\partial x} + \left(-\frac{3}{2} + \frac{|\mathbf{c}|^2}{2RT} \right) \frac{1}{RT} \frac{\partial RT}{\partial x} \right] \quad (81)$$

It is easiest to evaluate the integrals in components. As an example, one term is

$$\begin{aligned} & \int (c_x)^2 \frac{|\mathbf{c}|^2}{2RT} \frac{n}{(2\pi RT)^{3/2}} \exp\left(-\frac{|\mathbf{c}|^2}{2RT}\right) d\mathbf{c} = \\ & \int (c_x)^2 \frac{c_x^2 + c_y^2 + c_z^2}{2RT} \frac{n}{(2\pi RT)^{3/2}} \exp\left(-\frac{c_x^2 + c_y^2 + c_z^2}{2RT}\right) dc_x dc_y dc_z = \\ & \frac{5}{2} nRT \end{aligned} \quad (82)$$

The last line was obtained using standard integral tables.

The heat flux integral is evaluated using polar coordinates, as in Eq. (78)

$$\begin{aligned} & \int_0^\infty c^2 dc \int_{-1}^1 d\cos\theta \left[D(0; c, \boldsymbol{\Omega}) \frac{c^2}{2} c \cos\theta \right] = \\ & -\frac{1}{\sigma RT} \frac{\partial RT}{\partial x} \int_0^\infty c^2 dc \int_{-1}^1 d\cos\theta \left[M_1 \cos\theta \left(-\frac{5}{2} + \frac{|\mathbf{c}|^2}{2RT} \right) \frac{c^2}{2} c \cos\theta \right] = \\ & -\frac{1}{\sigma RT} \frac{\partial RT}{\partial x} \frac{2}{3} \frac{1}{(2\pi RT)^{3/2}} \int_0^\infty c^2 \exp\left(-\frac{c^2}{2RT}\right) \left(-\frac{5}{2} + \frac{c^2}{2RT} \right) \frac{c^2}{2} c dc \end{aligned} \quad (83)$$

The angular integral is elementary and the integral over c is again found in integral tables. The final result is shown in Eq. (79).

6 Gas mixtures

TO BE CONTINUED...?

THEN DO THE JUMP IN N AND RT.

DEAR READERS,

THIS IS AN OPEN-ENDED NOTE. WE WELCOME ANY AND ALL PEOPLE WHO WANT TO CONTRIBUTE AND COLLABORATE WITH US. THE LIST OF AUTHORS CAN BE EXPANDED, ANY WILLING CONTRIBUTOR CAN BE ADDED TO IT.

A MORE IMPORTANT REQUEST IS TO TRY TO THINK ABOUT THE IMPLICATIONS AND EXTENSIONS OF THE WORK. ONE EXAMPLE IS THE DERIVATION OF OTHER TRANSPORT COEFFICIENTS AND FLUCTUATION - DISSIPATION THEOREMS.

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